

# Certificate of Analysis

**Product Name:** S 32212 hydrochloride

**Catalog No.:** 4508

**Batch No.:** 1

CAS Number: 847871-78-7

IUPAC Name: 1,2-Dihydro-N-[4-methoxy-3-(4-methyl-1-piperazinyl)phenyl]-3H-benz[e]indole-3-carboxamide hydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{25}H_{28}N_4O_2 \cdot HCl \cdot \frac{1}{4}H_2O$

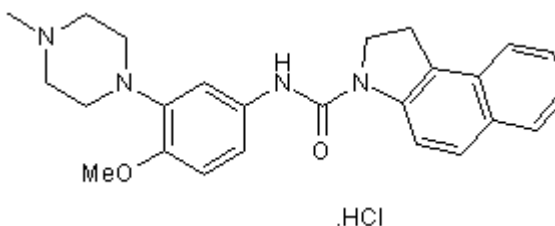
**Batch Molecular Weight:** 457.48

**Physical Appearance:** Pink solid

**Solubility:** water to 25 mM  
DMSO to 25 mM

**Storage:** Desiccate at RT

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.38$  (Dichloromethane:Methanol:Ammonia soln. [9:1:0.1])

**HPLC:** Shows 99.9% purity

**$^1H$  NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

|             | Carbon | Hydrogen | Nitrogen | Chlorine |
|-------------|--------|----------|----------|----------|
| Theoretical | 65.64  | 6.5      | 12.25    | 7.75     |
| Found       | 65.44  | 6.38     | 12.24    | 8.03     |

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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**Description:**

Inverse agonist of 5-HT<sub>2C</sub> receptors (pK<sub>i</sub> = 8.18 at human 5-HT<sub>2C</sub> INI receptors). Also an antagonist of human α<sub>2</sub>-adrenoceptors. Displays negligible affinity for α<sub>1A</sub>-adrenoceptors, histamine H<sub>1</sub> receptors and muscarinic M<sub>1</sub> receptors.

**Physical and Chemical Properties:**

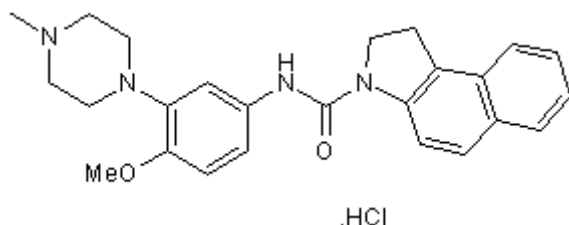
Batch Molecular Formula: C<sub>25</sub>H<sub>28</sub>N<sub>4</sub>O<sub>2</sub>.HCl. ¼H<sub>2</sub>O

Batch Molecular Weight: 457.48

Physical Appearance: Pink solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**Storage:** Desiccate at RT

**Solubility & Usage Info:**

water to 25 mM  
DMSO to 25 mM

**Stability and Solubility Advice:**

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

**SOLIDS:** Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

**SOLUTIONS:** We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

**References:**

**Millan et al (2012)** S32212, a novel serotonin type 2C receptor inverse agonist/α<sub>2</sub>-adrenoceptor antagonist and potential antidepressant: I. A mechanistic characterization. *J.Pharmacol.Exp.Ther.* **340** 750. PMID: 22178752.

**Dekeyne et al (2012)** S32212, a novel serotonin type 2C receptor inverse agonist/α<sub>2</sub>-adrenoceptor antagonist and potential antidepressant: II. A behavioral, neurochemical, and electrophysiological characterization. *J.Pharmacol.Exp.Ther.* **340** 765. PMID: 22178753.

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